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Title: ASC Directions in Machine Learning @LANL

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ASC Directions in Machine Learning @LANL

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Machine Learning For ASC

Goal: To find ways to impact ASC work in the IC, V&V and PEM.

In particular *in-line* ML as opposed to post processing.

We have more mature work in the CSSE/FOUS area of ASC

Existing work in Machine Learning

- **Image and Video based work (Dwave, Neuro, GPU, CPU)**
  - Sparse Coding/Compressive Sensing of Radiographic Sequences
  - Predicting Fractures with Sparse Coding
- **Infrastructure to run ML kernels on system log data Machine Learning on System Logs**
  - Developing tool to use temporal characteristics of system logs (including telemetry / environmental data)
    for anomaly detection
  - Developing tool to predict job outcome based on early warnings from system logs
  - Test developed DRAM fault mitigation tool on Trinity supercomputer

New starts for Machine Learning in Mid FY18

- **ML for Coarse-Graining and Structure Tagging for Fluid Simulations**
  - First goal - Predict future state of system by learning exact relationship of data at future times from data at previous times using data from simulation. Using Burger's equation.
  - Second goal - Learn approximate relationship of data at future times from coarse grained data at previous times using data from simulation

A Machine Learning Approach to Coarse-Graining and Structure Tagging for Fluid Simulations

Basic Idea: Learn how to integrate a fluid equation from simulation data

$$u_j^{n+1} = f(\ldots, u_{j-1}^n, u_j^n, u_{j+1}^n, \ldots)$$

Given data

Learn dependence

Method for learning dependence: Machine learning - use optimization to find parameters of a general non-linear transformation

New starts for Machine Learning in Mid FY18 (cont.)

- **ML for Multi-scale Materials**
  - *On-line* or *active* machine learning using inexpensive coarse-scale models combined in a single application code with expensive fine-scale models to simulate physical phenomena scalablely across multiple time and length scales.
  - PEM/ATDM effort
- **Developing ideas in V&V and Data reduction/analysis.**

Predicting Fractures with Sparse Coding

Example frame from fracture dataset

Goal: Predict unseen frames of a fracture propagation simulation by leveraging the latent representation learned by an unsupervised sparse autoencoder

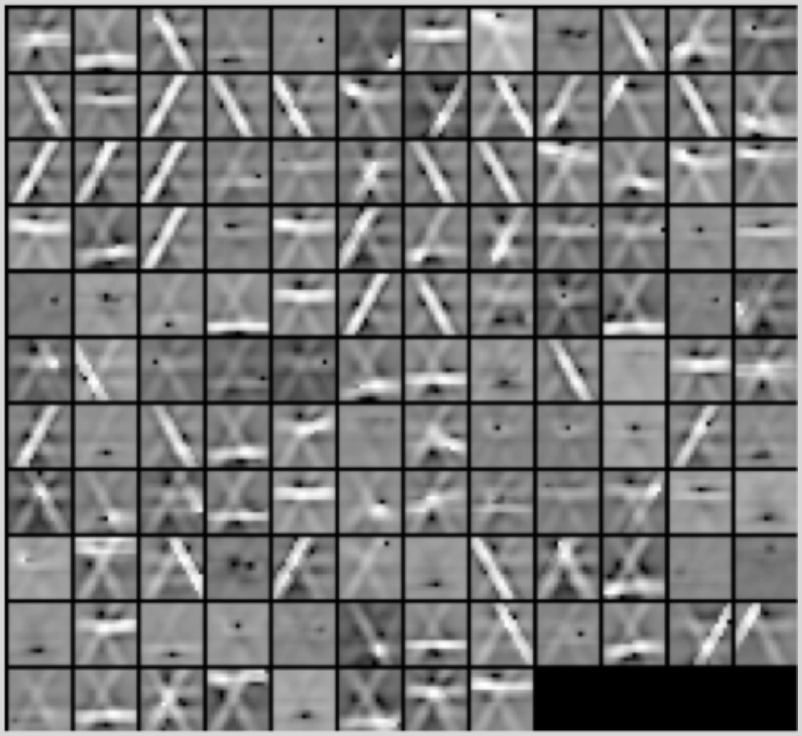
Predicting Fractures with Sparse Coding

Process: Train a sparse code on 12 difference frames of fracture propagation. Train a deep network to predict the full 24 frame sequence, using the sparse code as input.

Left: Actual data
Right:Predicted data

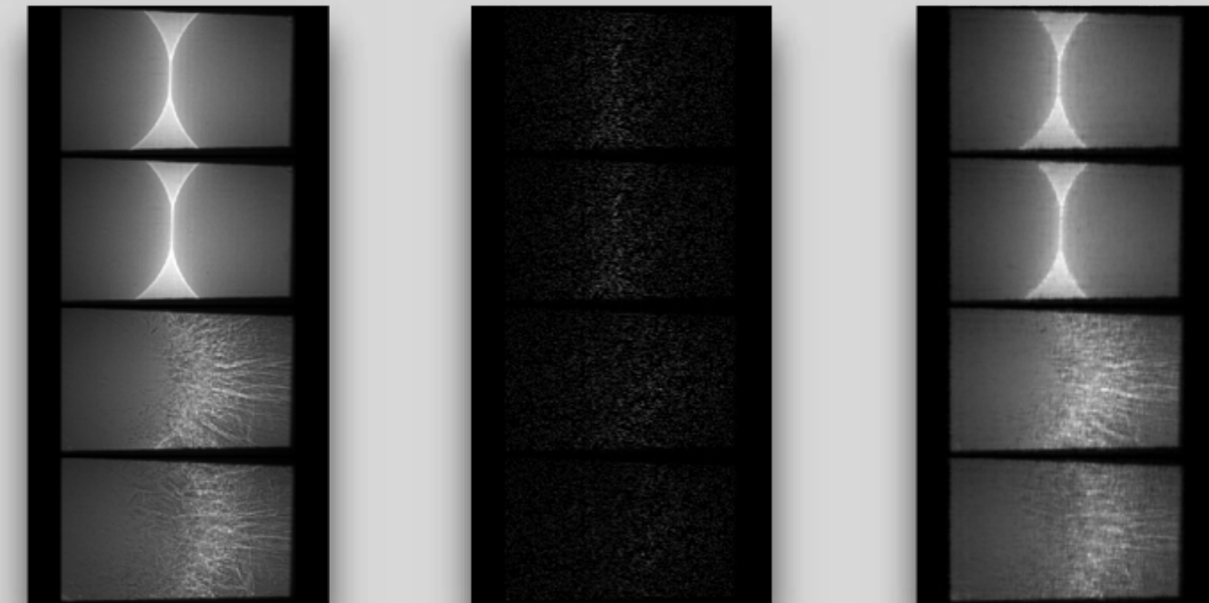
Predicting Fractures with Sparse Coding

Deep network weight visualization:



Reconstruct an X-ray image from random pixel sampling

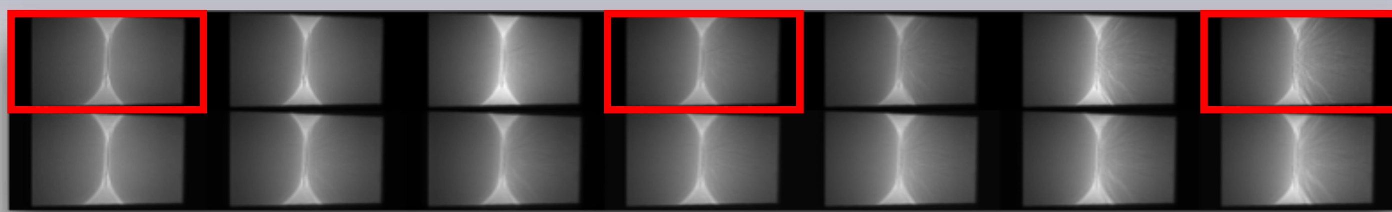
Masks cover 90% of pixels



(a) originals (b) masked samples (c) reconstructions

Z. Wang, O. Iaroshenko, S. Li, T. Liu, N. Parab, W. W. Chen, P. Chu, G. Kenyon, R. Lipton, and K.-X. Sune. Random on-board pixel sampling (ROPS) X-ray camera, Journal of Instrumentation (submitted)

Reconstruct intermediate frames (increase frame-rate)



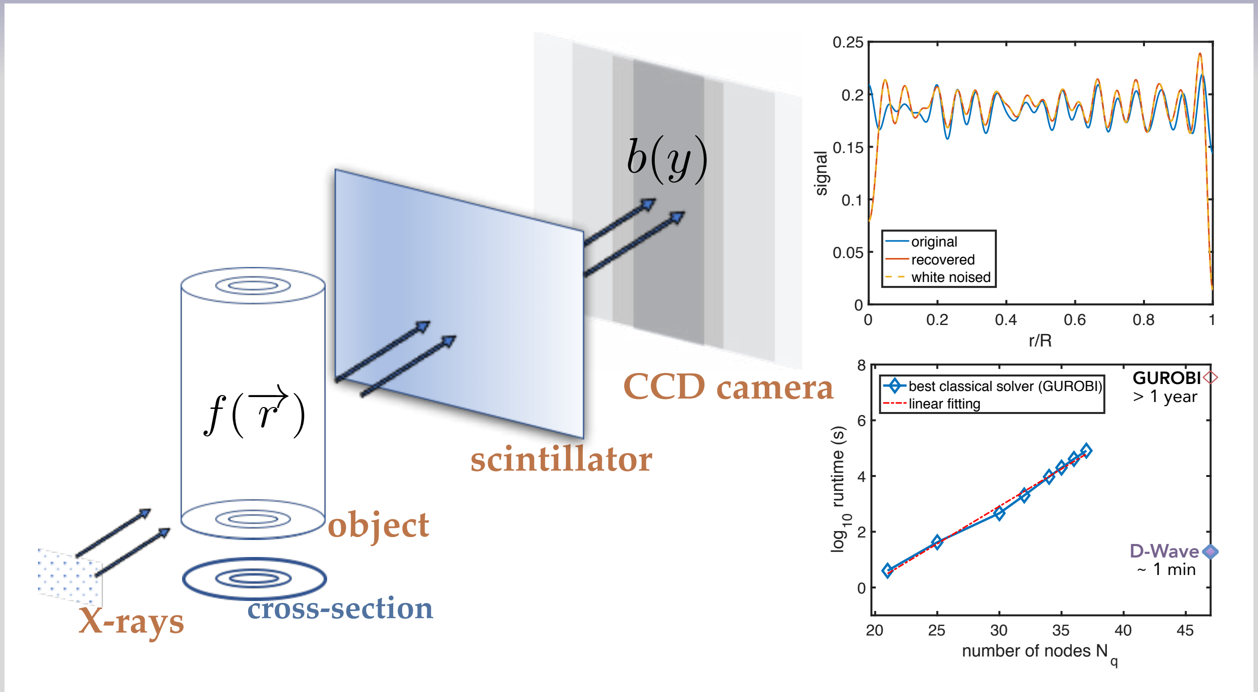
Top row: original frames, bottom row: reconstructed frames

Sparse coding algorithm can see only every third frame (red boxes)

			F_1	F_2	F_3	F_4	F_5	F_6	F_7		
N_1	D_1	D_2	D_3	D_4	D_5	D_6	D_7	D_8	D_9		
N_2		D_1	D_2	D_3	D_4	D_5	D_6	D_7	D_8	D_9	
N_3			D_1	D_2	D_3	D_4	D_5	D_6	D_7	D_8	D_9

Iaroshenko, O., Wang, Z., Watkins, Y. and Kenyon, G.T., Increasing frame rate of X-ray videos using spatiotemporal Dictionaries, workshop on *Deep Learning for Physical Sciences, NIPS 2017* (submitted).

Radiographic Inference



Nguyen, N.T.T., Larson, A.E., Kenyon, G.T., Implementation of a compressive sensing protocol on the quantum D-Wave 2X for inferring radial density profiles from synthetic radiographic images, (submitted)
Nguyen, N.T.T., Larson, A.E., and Kenyon, G.T., Generating sparse representations using quantum annealing: Comparison to classical algorithms, *IEEE International Conference on Rebooting Computing (ICRC),* 2017 (in press)